Continued Development of 4D-Variational Data Assimilation and Adjoint-Based Methods of Sensitivity Analysis and Applications Using ROMS

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LONG-TERM GOALS

The scientific goals of this research project are:

1. To explore the factors (e.g. uncertainties in initial conditions versus those in surface forcing and boundary conditions) that limit the predictability of the circulation in regional ocean models in a variety of dynamical regimes;

2. To compare two state-of-the-art variational data assimilation strategies (4DVAR and IOM) and gain experience using both in regional ocean models;

3. To develop ensemble prediction techniques for regional ocean models;

4. Demonstrate the utility of the ROMS data assimilation framework in a real-time, sea-going environment for prediction studies in the Intra-Americas Sea (IAS) with particular emphasis in the Caribbean Sea. As such, we will demonstrate, as a proof of concept, the utility of adjoint modeling and 4DVAR data assimilation in a real-time operational setting, at sea.

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OBJECTIVES

The main objectives are: (**i**) to develop real-time data assimilation and prediction techniques for the coastal oceans and semi-enclosed seas, with particular emphasis on the IAS and U.S. west coast, based on continuous satellite-based and in-situ upper ocean monitoring systems; (**ii**) to demonstrate the utility of variational data assimilation in real-time, and in a sea-going environment; (**iii**) to demonstrate the value of collecting routine ocean observations from existing coastal ocean observing systems and specially equipped ocean vessels; and (**iv**) to develop much needed experience in both the assimilation of disparate ocean data and ocean prediction in regional ocean models using sophisticated variational data assimilation techniques.

APPROACH

The primary tool used is the Regional Ocean Modeling System (ROMS) and the Terrain-coordinate Ocean Modeling System (TOMS). This is a collaborative effort involving Drs. Arthur Miller and Bruce Cornuelle at the Scripps Institute of Oceanography, Dr. Hernan Arango at Rutgers University of New Jersey, Dr. Emanuele Di Lorenzo at the Georgia Institute of Technology, and Dr. Ralph Milliff at Colorado Research Associates. To address the aforementioned goals and objectives, we are using a recently developed suite of tools that utilize the tangent linear (TL), adjoint (AD), and finite-amplitude tangent linear (RP) versions of the ROMS/TOMS code. ROMS, TLROMS and ADROMS were developed under the support of previous ONR funding, while the development of RPROMS was supported by NSF.

As part of this effort we have also developed several toolkits that utilize the various versions of ROMS. These include: (1) a Generalized Stability Theory (GST) toolkit; (2) an adjoint sensitivity analysis toolkit; and (3) a suite of 4-dimensional variational data assimilation platforms that include strong constraint incremental 4DVAR (IS4DVAR), an indirect representer-based weak constraint 4DVAR (W4DVAR), and a weak constraint Physical Space Analysis System (W4DPSAS). W4DVAR is based on the Oregon State University Inverse Ocean Model (IOM) of which ROMS is also a component via a separate NSF funded effort (DiLorenzo et al, 2007; Muccino et al, 2007). Our primary efforts during the last 12 months have involved implementation and development of a real time ROMS IS4DVAR data assimilation and ensemble prediction system for the IAS that is run onboard the Royal Caribbean Cruise Line (RCCL) vessel *Explorer of the Seas* (Powell et al, 2007a,b). In addition, we have invested considerable time and effort in the continued development and improvement of all the ROMS 4DVAR algorithms, particularly with regard to preconditioning of the conjugate gradient descent algorithms.

WORK COMPLETED

During the current reporting period we have completed the following tasks:

(1) **Sea-trials of a real time IAS ROMS data assimilation and ensemble prediction system aboard the RCCL *Explorer of the Seas***. The real time system consists of the following components:

    (i)   IS4DVAR was run on a 40km grid using a 14 day assimilation window. All available satellite SST, SSH and shipboard ADCP data were asssimilated into IAS ROMS to

generate a model initial condition for the current day. The first-guess/background initial condition used during each assimilation cycle was the ocean state at the end of the previous data assimilation cycle. During each assimilation cycle, the model was forced with a blended surface wind product computed by Ralph Milliff and Jan Morzel at CoRA using satellite scatterometer winds and NCEP reanalyses. In addition, NCEP reanalyses were used to provide near-surface meteorological conditions for computing surface heat and fresh water fluxes for ROMS. Data assimilation cycles were repeated every 3-7 days depending on the availability of new observational data.

(ii) A 51 member ensemble of IAS forecasts of 14 days duration were run starting from the ocean state estimates derived from IS4DVAR. One of the ensemble members consisted of a control forecast initialized with the IS4DVAR initial condition from (i), and forced with the surface momentum, heat and freshwater fluxes derived from an extended range NCEP forecast product. Individual ensemble members were derived by perturbing the model initial conditions and surface wind forcing within the limits of the expected uncertainties. The initial condition perturbations were derived from the IS4DVAR assimilation cycle and consisted of orthonormalized increments from each inner-loop that were used to generate 25 independent perturbations. Each perturbation was used twice with a positive and negative amplitude. The surface wind stress was perturbed using a Bayesian Hierarchical Model (BHM) for the IAS surface winds. The IAS BHM was developed by Alessandro Bonazzi during a 6 month visit to UC Santa Cruz. Alessandro is a graduate student working with Prof. Nadia Pinardi at the University of Bologna and with Ralph Milliff at CoRA on BHM methods in the Mediterranean Sea, work that is also supported by ONR. The IAS BHM was trained using NCEP reanalyses and satellite scatterometer winds, and was used to generate 50 independent, physically realizable surface wind fields that were used to generate ensemble members, in conjunction with the initial condition perturbations.

(iii) The IS4DVAR and ensemble prediction system was also run using a 20km version of IAS ROMS. The 40km IS4DVAR solution interpolated onto the 20km grid was used as a first-guess/background initial condition for the 20km IS4DVAR so as to minimize the computational effort required to assimilate the observations into the model, a computationally demanding task at 20km resolution.

(iv) The entire IS4DVAR and ensemble prediction system outlined in (i), (ii) and (iii) involves many stages and is quite complex, and was managed by a series of carefully constructed Unix scripts as illustrated in Fig. 1. During the sea trials (described in (2)) the Unix scripts were run manually by project personnel aboard the ship. Later, the Unix scripts were fully automated so that the system was capable of running with the minimum of supervision.

(v) The entire system was run on a dedicated 4 CPU computer installed in the OceanLab (http://www.rsmas.miami.edu/rccl/basic.html) aboard the *Explorer*.

(vi) Ensemble forecast products were automatically generated and uploaded to a project website, http://www.myroms.org/ias/archive_fine.php.

(2) **Real time forecasting at sea.** Initial sea trials of the system described in (1) were conducted aboard the RCCL *Explorer of the Seas* during the period 7 January – 18 February, 2007.

During this 6 week period, the cruise ship alternated between the two routes shown in Fig. 2. During weeks 1, 3 and 5 the ship plied the so-called "eastern track" (Miami to St Thomas, U.S. Virgin Islands), and during weeks 2, 4 and 6 it travelled the "western track" (Miami to Belize). During each cruise leg, the *Explorer* made continuous measurements of the ocean velocity field to a depth of 1000m using two hull-mounted ADCP units. During a typical 2 week period, *Explorer* crosses several major passages bordering the northern Caribbean, traverses the Florida Current and Yucatan Current in several locations, and crosses the Yucatan Channel several times. Each week 1 or 2 project personnel (Powell, Moore, Milliff, Morzel and Chhak) were present onboard the ship to run the real time system described in (1). During this initial 6 week trial period, project personnel experimented with different configurations of the system. At the end of the 6 week period this information was used by the PIs to configure an optimum system that would be run fully automated as described in (4).

(3) **Education and outreach.** While onboard the *Explorer of the Sea*, project personnel also participated in an important education and outreach program run and managed by the Rosenstiel School of Marine and Atmospheric Sciences (RSMAS) at the University of Miami. Each week a member of our project team gave two general science talks to the passengers onboard *Explorer* (see http://www.rsmas.miami.edu/rccl/schedule.html) and conducted ~ a dozen guided tours of the onboard instrument and laboratory facilities. An integral component of the OceanLab tour included a live, real time display of the IAS ROMS forecast information as it was running onboard the ship. A mirror of this display can be found at http://www.myroms.org/ias/ by selecting the "Lab Tour" menu item on the left – "coarse" shows the 40km products and "fine" the 20km case. An example screen capture image is shown in Fig. 3. Participating in the onboard education and outreach program gave us the opportunity to showcase our ONR project, and talk with the passengers about the importance and applications of ocean forecasting. During the 6 week trial period we estimate that we personally interacted with ~1,500 passengers. However, since Feb. 2007, the real time forecasting system has been running fully automated onboard *Explorer* and the live OceanLab display has continued to provide forecast information to passengers during the lab tours during the intervening 9 month period. Therefore, the exposure of this project to the public has been extensive.

(4) **Implementation of an automous data assimilation and ensemble prediction system at sea.** The real time IS4DVAR and ensemble prediction system described in (1) and tested at sea as described in (2) was configured to run fully automated in OceanLab aboard *Explorer*. Every 3.5 days, a new data assimilation and ensemble forecast cycle begins, and forecast information is automatically uploaded to the project website everyday (cf. Fig. 1). Because of delays in the release of real time SST and SSH observations displayed on the project web site are typically behind by a day or so.

(5) **Development of efficient preconditioned IS4DVAR algorithms.** IS4DVAR is a computationally demanding data assimilation procedure, and as model resolution increases the cost can be computationally prohibitive. It is therefore very important that the minimization algorithm used in the inner-loops of IS4DVAR be as efficient as possible. With this in view, we have invested a great deal of effort in implementing a minimization algorithm based on the Lanczos method. The Lanczos method has the particular advantage of allowing estimates to be made of the Hessian matrix (i.e. the cost function second derivative) as the minimization

proceeds. This information can be used to precondition subsequent outer-loops (and potentially future assimilation cycles if the observational array does not change substantially). The implementation that we have been using is based on the so-called CONGRAD algorithm developed at ECMWF and CERFACS in France. The PIs have maintained a close working relationship with algorithm developers at ECMWF and CERFACS which has proved very fruitful for this and other projects. Implementation and testing of CONGRAD in the ROMS IS4DVAR continues, and a variant of the method is also being used in the W4DVAR and W4DPSAS algorithms. In addition, Hessian matrix estimates obtained using CONGRAD can be used to estimate the analysis error of the resulting 4DVAR ocean state estimates (Powell and Moore, 2007), and can be used to design more optimal observing networks.

(6) **Data assimilation using a multi-resolution approach.** Our experiences in the real time IAS ROMS data assimilation and ensemble prediction arena have highlighted the need for a multi-resolution approach to data assimilation in the ocean. The basic idea is to perform IS4DVAR on a sequence of grids with ever increasing horizontal (and perhaps vertical) resolution. The optimum ocean state estimate derived from one grid is used as the first-guess/background initial condition constraint for IS4DVAR on the next highest resolution grid. In this way the large-scale circulation features in the observations are captured on the low resolution grid at relatively low computational expense. These features are then passed to the next grid with higher resolution, and further cycles of IS4DVAR not only refine the large-scale circulation estimate, but also begin to recover details of the observed mesoscale flow features which develop on the large-scale environment. Assimilating on progressively higher resolution grids should refine the estimates of the ocean mesoscale and large-scale even further, while at the same time resolving and recovering smaller-scale features that may be present in the observations. We have experimented with this approach in the IAS using the 40km and 20km ROMS grids, and plan to include a 10km grid in the IAS IS4DVAR procedure.

(7) **Balancing operators.** The current ROMS IS4DVAR system is limited in its capacity to use multivariate covariance information in its estimates of the ocean state. Work has recently begun to include fully multivariate covariance information by decomposing the circulation into balanced (i.e. geostrophic) and unbalanced (i.e. ageostrophic) components. IS4DVAR proceeds to minimize the cost function by adjusting the unbalanced circulation, following experience and methods developed in numerical weather prediction and in oceanography at CERFACS.

RESULTS

Prior to running the real time system onboard *Explorer of the Sea,* an extensive series of experiments and tests of the IS4DVAR system were performed. These are described in detail by Powell et al (2007a). By way of an illustration of the efficacy of the IS4DVAR system, Fig. 4 shows a comparison of the root mean square error (RMSE) in SST for two experiments: **ExN** where no data were assimilated, and the model was forced only with our best estimate of the surface forcing; and **ExAV** where all available SST, SSH and *Explorer* ADCP were assimilated into the model every 14 days using a 14 day data assimilation window. The RMSE were computed for the period 1 Jan 2005 to 28 Feb 2007. Comparing Fig. 4(a) with Fig. 4(c) reveals that data assimilation significantly reduces the RMSE error in SST over most of the model domain. However, Fig. 4(c) also reveals that there are areas in which the SST error remains relatively high even in the presence data assimilation, such as the

Loop Current extension, coastal areas of the Gulf of Mexico, and the upwelling region along the coast of Venezuela.

Also shown in Fig. 4 (b and d) are variations in the temporal correlation (TC) between the model SST and observed SST during each 14 day period for 1 Jan 2005 to 28 Feb 2007 for the same two experiments. Figures 4c and 4d indicate that despite the elevated RMSE in the aforementioned regions, the temporal variations in SST are captured reasonably well when data are assimilated.

The impact of assimilating shipboard ADCP from *Explorer of the Seas* is illustrated in Fig. 5 which shows the RMSE (panels a and c) and the anomaly correlation (ACC) between the model and observations (panels b and d) for the zonal and meridional components of velocity for various experiments, including ExN and ExAV. The RMSE and ACC in this case are computed for the entire Gulf of Mexico and Caribbean Sea. The results from a third experiments, **ExAVS,** are also shown in which only SST and SSH data are assimilated. Comparing the curves for ExAV and ExAVS, Fig. 5 indicates the positive impact that assimilating ADCP data has on the velocity along the cruise tracks. Comparing ExN and ExAVS shows that assimilating only SST and SSH leads to no significant improvement in the circulation along the cruise tracks.

The statistics that are used to characterize the error in the first-guess/background initial condition of IS4DVAR have a significant impact of the efficacy of the data assimilation circulation estimates. When we begin a new data assimilation experiment, the model solution from a forced integration of the model is used as the first-guess/background. In this case, the relevant background error statistics are those of the model climatology, because on average the difference between the forced model solution and the observations is the same as the difference between two randomly chosen states. However, after a few data assimilation cycles, the first-guess/background state (which recall is taken from the previous assimilation cycle) is much closer to the observations than climatology. In this case, the climatological statistics are no longer a valid description of the uncertainties in the background – in actual fact the background is more accurate than climatology. Figure 6 shows the impact of updating the statsitics of the background error covariance matrix during experiment ExA, very similar to ExAV described above. The parameter shown in Fig. 6 is a measure of the theoretical minimum value of the IS4DVAR cost function, and the desired value is 1. The second experiment, **ExANmc**, shown in Fig. 6 is for the case where the background error statistics are updated in May 2005 using the so-called "NMC method", commonly used in numerical weather prediction. The positive impact of updating the background error statistics on the system is cleary evident in Fig. 6.

In Table 1, a comparison of the transport through the Yucatan Channel, the mean and standard deviation. The observed transport is ~24Sv. Without data assimilation (ExN) the model transport is ~26Sv, while with data assimilation (ExA and ExAV) the transport is closer to that observed. In all cases though, the Yucatan Channel transport standard deviation is significantly larger than observed.

Results from the real time data assimilation ensemble prediction period, 7 Jan 2007 to the present, are shown in Fig. 7. The panels on the left show the 14 day average rms error in SST and SSH from each data assimilation cycle (red curve) and for 14 day control forecast initialized using the initial condition from the previous data assimilation cycle. On average, the SST error during the data assimilation cycle is ~0.4C and increases to only ~0.5C during the forecast interval. Similarly, the average SSH error is ~7cm during the data assimilation cycle and increases to ~8cm during the forecasts. Clearly, however, there is considerable variation in the growth of forecast errors from one forecast period to the next, and

we are working to understand the factors that control these variations. Also shown in Fig. 7 (right panels) are the pattern correlations between the model SST and SSH fields and the corresponding observed fields. The pattern correlations for SST are generally high during the entire period during both the data assimilation and forecast phases. On the otherhand, the pattern correlations for SSH are lower and generally below 0.6 for the forecasts. The lower pattern correlations of SSH are we believe associated with the univariate nature of the background error covariance statistics that are used by current version of ROMS IS4DVAR. Our hope is that these issues will be alleviated by the introduction of the balanced operators described in (7) above.

IMPACT/APPLICATIONS

The IAS component of the project has demonstrated the utility of ROMS variational data assimilation algorithms in a real-time, sea-going environment. Specifically we have demonstrated that a sophisticated, state-of-the-art ocean model, data assimilation, and ensemble prediction system can be used in a sea-going environment by non-expert users. The latter was demonstrated by the fact that two of the project personnel who participated in the sea trials described in (2) above, namely Jan Morzel and Kettyah Chhak, are not data assimilation experts, and neither had any prior knowledge of the ROMS IS4DVAR and ensemble prediction before their respective cruises. However, despite this, both Morzel and Chhak were able to successfully run the system using a set of simple instructions provided by Powell. Furthermore, the transition of the system to a fully autonomous state running onboard *Explorer of the Seas* demonstrates that a well designed and sophisticated system like that described here can be run remotely at sea with minimum operator intervention. The real time IAS ROMS data assimilation and ensemble prediction system developed as part of this project will form the basis of similar systems proposed for the U.S. west coast and the California Current system.

Our experiences with the IAS real time system have highlighted a number of important issues in relation to real time data assimilation and prediction in general. One of the major issues that we had to contend with was the timeliness and availability of both quality controlled ocean observations, and ocean forcing products from atmospheric forecast models. With regard to ocean observations, the quality of available real time products for SST (and SSH) varies considerably, and in general the differences between products are as large as the difference between the model forecast and any individual product. With regard to atmospheric forecast model products required to run an ocean forecast, these presented the greatest challenge in real time. First of all, only a low resolution (~ 2 degrees) operational product is available for the entire IAS region from NCEP, and the quality of the extended range 14-day forecast product beyond the first 2 or 3 days is questionable. Second, because of bandwidth problems at NCEP, the availability of the extended range forecast product cannot be guaranteed. In fact, during week 3 of the sea trials in early February, the extended range product was unavailable for several days. All of these issues combined indicate that for serious real time ocean forecasting efforts to become a reality, further improvements and advances need to be made in the real time delivery of quality controlled ocean observations and atmospheric forecast products.

Finally, we note that the impact of the ongoing education and outreach component of this project may be considerable. As noted above in (2), project personnel have interacted with the general public and have showcased not only the importance of this project, but also the importance of the type of research that is supported by ONR. These efforts continue with the live ROMS IAS forecast display, now an integral component of the OceanLab tours for passengers aboard *Explorer*.

TRANSITIONS

The various ROMS toolkits and 4DVAR data assimilation algorithms are all available from the Rutgers website and are being actively used and further developed by other research groups in the U.S. To facilitate this transition a second mini-workshop on the ROMS data assimilation platforms was held at the University of California Santa Cruz in Summer 2007 and attended by students, post-docs and other researchers from Rutgers University, Scripps, Georgia Institute of Technology, University of Colorado, CICESE and UC Santa Cruz.

RELATED PROJECTS

The work described here is intimately related to the following ONR supported projects::

"ROMS/TOMS Tangent Linear and Adjoint Models: Data Assimilation Tools and Techniques", PI Hernan Arango, grant number N00014-00-1-0227.

"ROMS/TOMS Tangent Linear and Adjoint Models: Data Assimilation Tools and Techniques ", PIs Arthur Miller and Bruce Cornuelle, grant number N00014-99-1-0045.

"ROMS Data Assimilation Tools and Techniques",PI Emanuele Di Lorenzo, grant number N00014-05-1-0365.

"Bayesian Hierarchical Models to Augment the Mediterranean Forecast System", PI Ralph Miliff, grant number N00014-05-C-0198.

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None

PUBLICATIONS

Chhak, K.C., H.G. Arango, A.M. Moore and E. Di Lorenzo, 2006: An adjoint sensitivity analysis of Intra-Americas Sea to variations in surface forcing using ROMS. In preparation for submission to *Ocean Modelling* in winter 2007.

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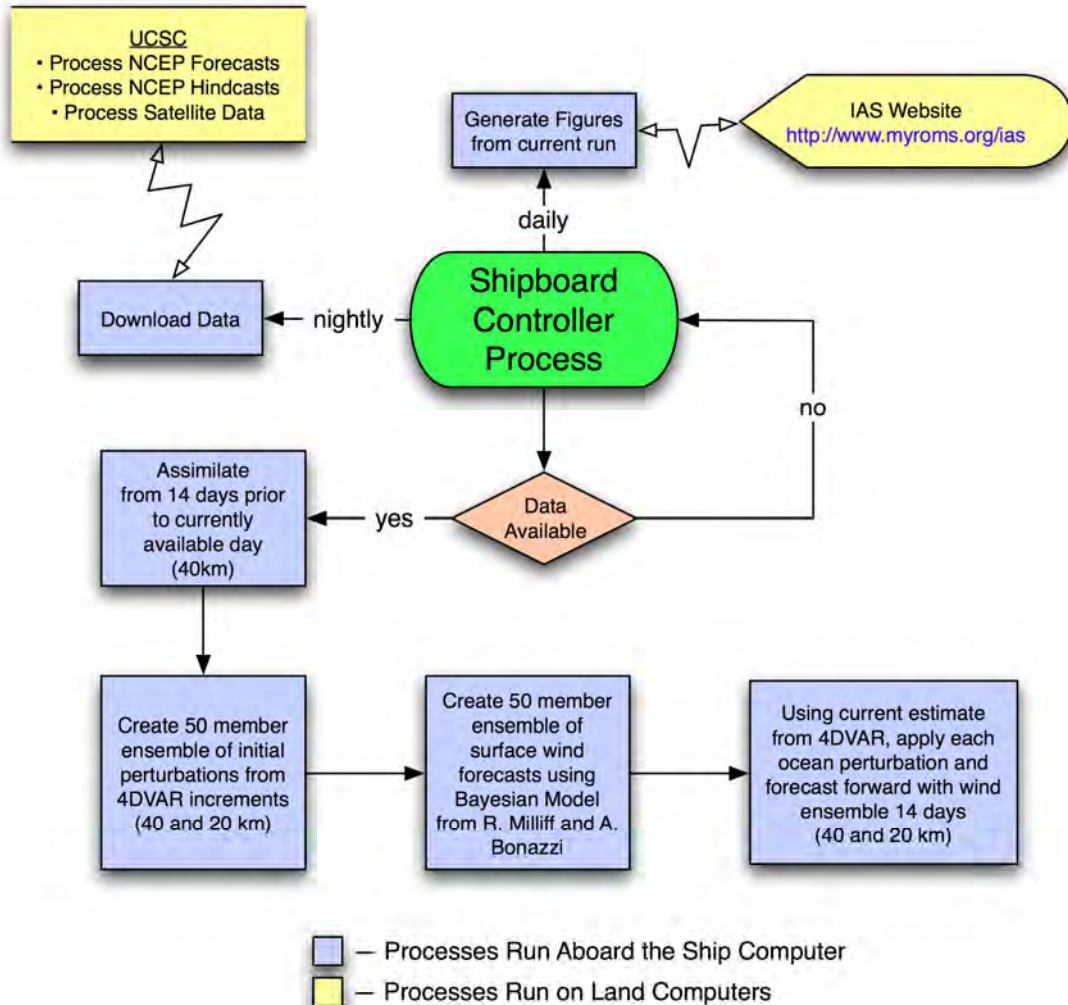
Figure 1: A flow chart outlining the real time IS4DVAR data assimilation and ensemble prediction system that is run onboard the Royal Caribbean Cruise Lines vessel Explorer of the Seas. In order ot reduce the volume of data that must be transferred to the computer system in the Explorer OceanLab, preliminary processing of ocean surface forcing data and observations occurs at UC Santa Cruz. The ROMS forcing and observation files are then transferred to the ship's computer which interrogates the UC Santa Cruz computer system at daily intervals, downloading any new data that is available.
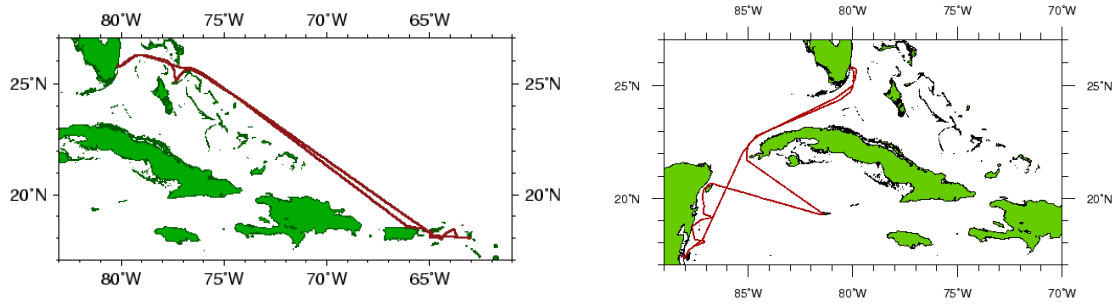
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Figure 2: The current Explorer of the Seas cruise tracks: eastern track (left) and western track (right).
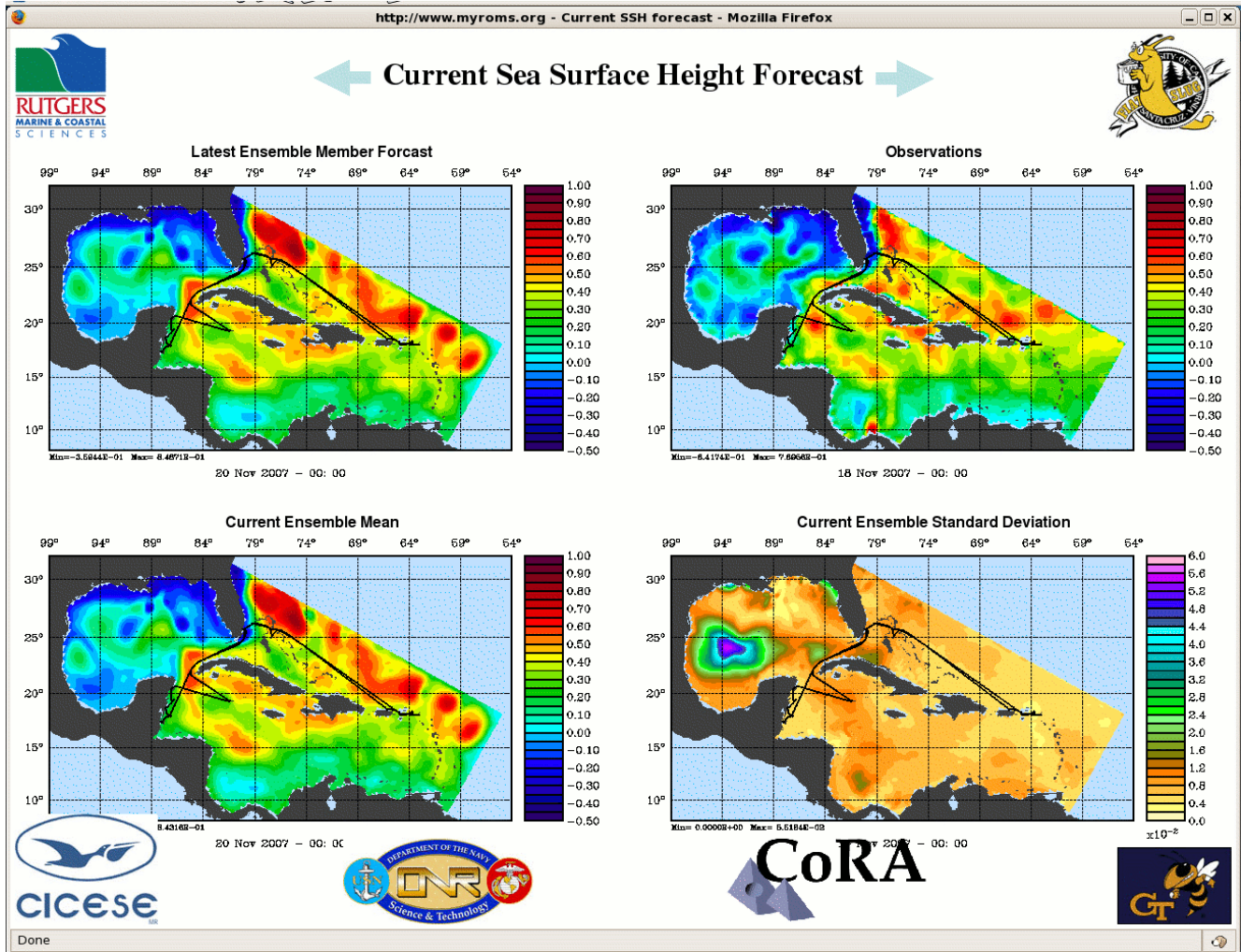

Figure 3: An example ensemble forecast product for 20 Nov 2007 generated by the 20km real time data assimilation and ensemble prediction system running onboard Explorer of the Seas. The upper left panel shows the forecast SST for the latest ensemble member, while the lower left panel shows the ensemble mean forecast for SST (i.e. the mean of all ensemble members that have run up to the current time). The spread in SST of the ensemble members about the ensemble mean is shown in the lower right panel, and is an indicator of forecast uncertainty. The observed SST is shown in the upper right panel. Because of the delay in obtaining real time observations, the observations shown are typically a day or so old
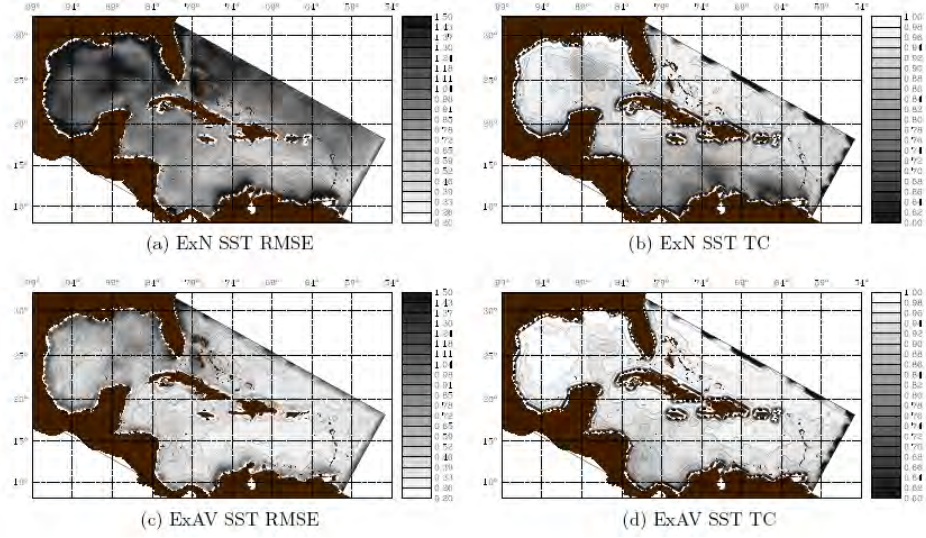
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Figure 4: Spatial maps of the root mean square error (RMSE) in SST and the temporal correlation (TC) between the model SST and observations for the two experiments ExN and ExAV.
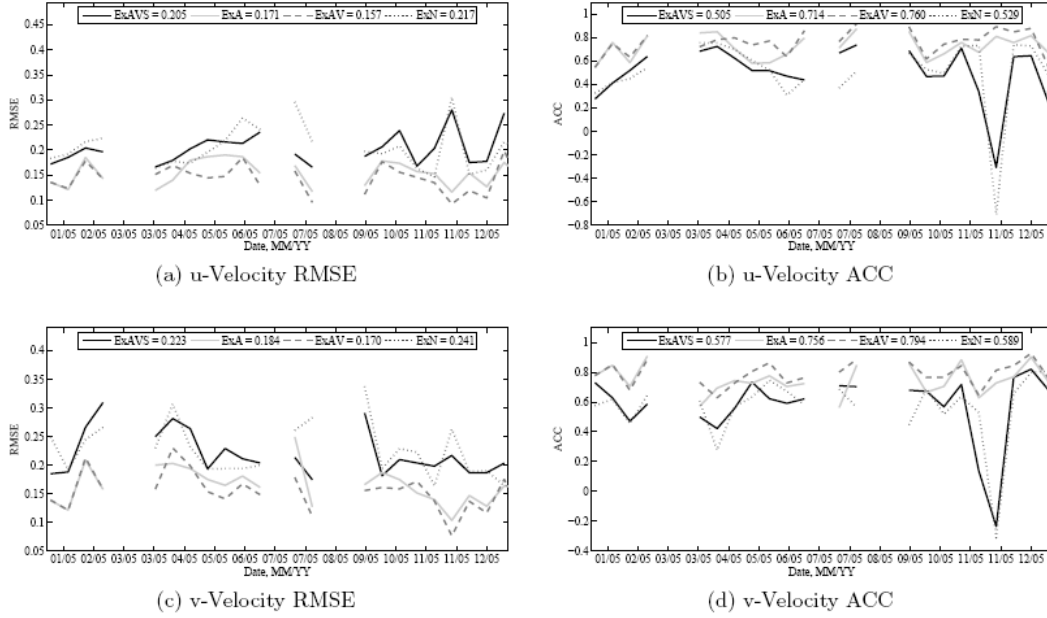

Figure 5: Timeseries of the root mean square error (RMSE) and the anomaly correlation (ACC) between the model and observations for zonal and meridional velocity for experiments ExN and ExAV.
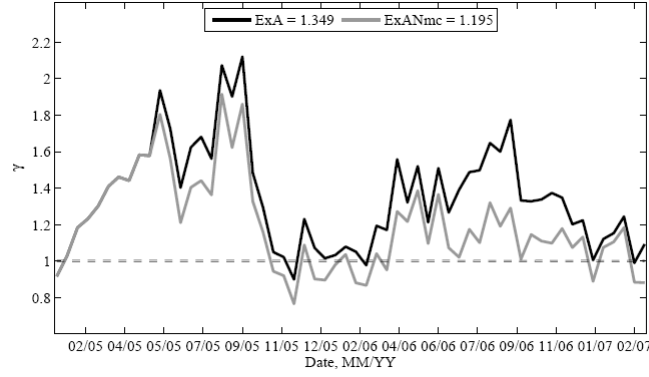
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Figure 6: A timeseries of γ, a measure of the theoretical minimum value of the IS4DVAR cost function, that results from using two different estimates of the background error covariance matrix. A value of γ=1 is desirable.

Table 1: A comparison of the Yucatan Channel transport, mean and standard deviation, from ExN, ExAV and observations (CANEK).

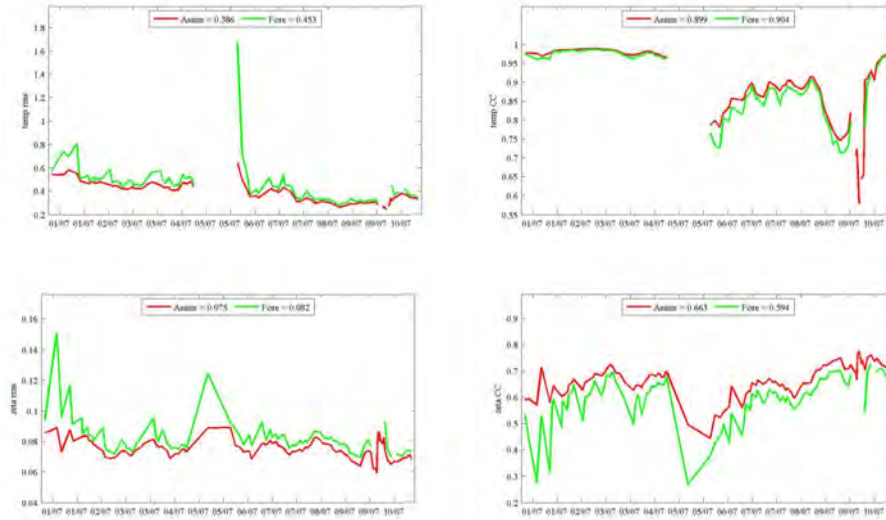|	CANEK	ExN	ExA	ExAV
Mean (Sv)	23.8	26.0	24.3	24.5
Std. Dev (Sv)	1.0	4.4	8.3	7.4

Figure 7: Timeseries of rms error in SST (top left) and SSH (bottom left) between the 40km model and observations for the real time forecast period 7 Jan 2007 to present. The red curve shows the average rms errors for each 14 day data assimilation cycle, and the green curve shows the average rms error of the resulting 14 day control forecast. Also shown are the pattern correlations between model SST and observarions (top right) and model SSH and observations (bottom right).